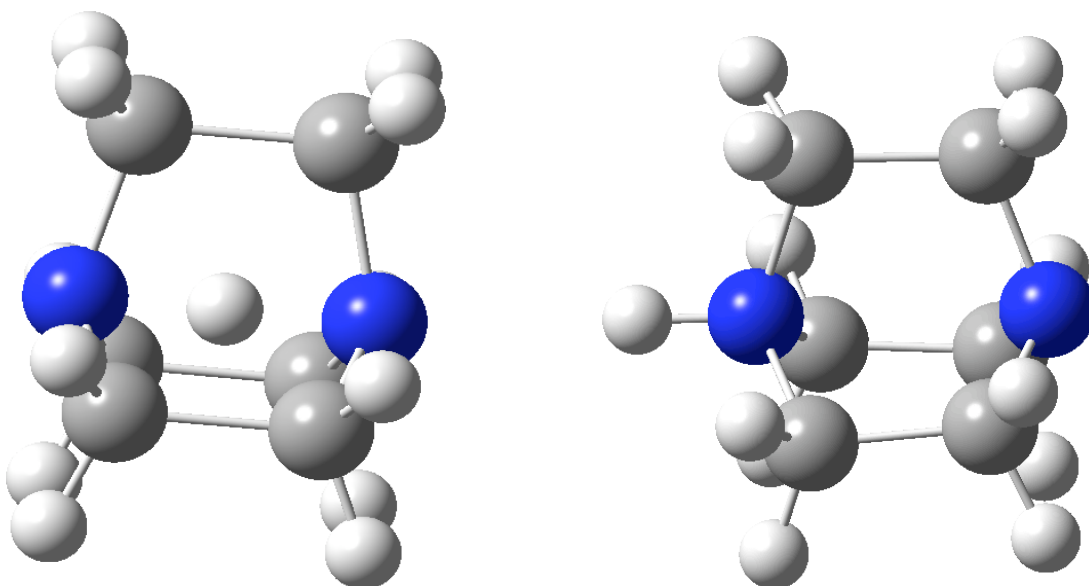


Strategic Removal of Triton and Tritium Oxide from Tritiated Water

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In order to solve the problem of tritiated water waste from nuclear power plants, different materials were tested to see their abilities to draw the triton (T⁺) or tritium oxide (OT⁻) that form tritiated water. We focused on the reaction between amines and analogs of Amberlite IRA 400 and Amberlite IR 96 SB with the tritiated water. Using Gaussian 03, the free energy for all the reactants and products were found. In order to conserve time, most calculations were made with different levels of electronic structure methods to compare and achieve a compromise between time and accuracy. The reaction change in free energy, including the solvation, were used to determine which material has the greatest capability to draw the triton (T⁺) or the tritium oxide (OT⁻).



Two macrobicyclic amines, the one on the left with a proton on the inside and the right with a proton on the outside.